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Off-center D^- centers in a quantum well in the presence of a perpendicular magnetic field: angular momentum transitions and magnetic evaporation

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We investigate the effect of the position of the donor in the quantum well on the energy spectrum and the oscillator strength of the D^- system in the presence of a perpendicular magnetic field. As a function of the magnetic field we find that when D^- centers are placed sufficiently off-center they undergo singlet-triplet transitions which are similar to those found in many-electron parabolic quantum dots. The main difference is that the number of such transitions depend on the position of the donor and only a finite number of such singlet-triplet transitions are found as function of the strength of the magnetic field. For sufficiently large magnetic fields the two electron system becomes unbound. For the near center D^- system no singlet-triplet and no unbinding of the D^- is found with increasing magnetic field. A magnetic field vs. donor position phase diagram is presented that depends on the width of the quantum well.

I. INTRODUCTION

In multilayer and quantum well structures, such as $GaAs/Al_xGa_{1-x}As$, the electrons bound to donor impurities situated in the barrier tend to migrate in the well, due to the favorable potential gap. There they are trapped by the impurity donors, such as Si, that are naturally or artificially present in the material. The trapping of one electron by a donor does not completely screen the charge of the donor itself, thus bounded states of negative charged donors are in principle and in practice possible.[1]

A great deal of attention has been given to the formation and stability of negative donor centers in semiconductors in recent years. Those systems, indeed, being the simplest many-body system, represent an interesting occasion to study the electron-electron interactions in solids.

In previous experimental and theoretical studies the dependence of the binding energy of the D^- on the magnetic field strength and on the dimension of the quantum well have been done. While a great part of these works consider the on-center D^- problem,[2–4] i.e. when the impurity donor is at the center of the well, the study of the off-center, i.e. when the impurity donor is displaced from the center of the well, and the barrier D^- problem, i.e. when the donor is in the barrier, are much less investigated. On the theoretical side, Zhu and Xu[5] studied the spin-singlet L=0 and the spin-triplet L=-1 states for a quasi-2D D^- while Fox and Larsen[6] studied the barrier D^- in which the electrons are moving in a perfect 2D plane. The dependence of the properties of a D^- system on the position of the donor with respect to the center has been partly investigated by Marmorkos *et al.*[7] They considered the problem of a double quantum well in which one of the two wells hosts, in its center, the donor, while the other contains the electrons. On the experimental side we point out the work of Jiang *et al.*[8] in which experimental evidence of an off-center D^- system was presented. All these studies on off-center and barrier D^- show spin-singlet spin-triplet transitions of the ground state with increasing strength of the magnetic field. But the situation studied in previous works differs from the real problem of the off-center D^-. The work of Zhu *et al.* is most close to the real experimental situation but they studied only the first two state of the D^- system. Such singlet-triplet transitions have also been observed in electron systems confined in quantum dots and are known as *magic magnetic number* ground state transitions.[11] In quantum dots the electrons are held together by a parabolic or hard wall confinement potential which for the D^- problem is replaced by the Coulomb potential of the donor impurity. Thus it seems that the appearance of singlet-triplet transitions is a characteristic feature of confined electronic systems, and in this paper we will shed more light on the condition under which such transitions appear in the D^- system. The D^- problem has the added flexibility that the singlet-triplet transition can be influenced by changing the position of the donor with respect to the center of the quantum well. It is even possible that for certain donor positions there is no singlet-triplet transition at all.

In the present paper we study the properties of the off-center D^- as function of the position of the donor in the well, and as function of the quantum well width in the quasi-2D approximation. In Sec. II we present our model and explain how we obtain the wave function and energy of the different D^0 and D^- levels. Next, in Sec. III, we present and discuss the energy spectral behavior for quantum wells of width 200Å and 100Å. Then, we compare the results of the two calculations in order to have a better understanding of the reasons that underlie the different behaviors of the two energy spectra. Next, in Sec. IV, we evaluate and study the dependence of the oscillator strength and of the transition energies on the magnetic field and on the position of the donor with respect to the center of the well. In Sec. V we use our model to explain the cyclotron resonance experiment of Jiang *et al.*[8] Our conclusions are presented in Sec. VI

II. THE MODEL

The properties of the off-center D^- in a finite-height quantum well under the influence of a perpendicular magnetic field will be treated in the present paper. In the frame of the effective mass approximation the Hamiltonian of the D^- system is given by

$$H_{D^-} = H_1^{D^0} + H_2^{D^0} + V_{ee}(|\vec{r}_1 - \vec{r}_2|), \tag{1}$$

where $H_i^{D^0}$ is the Hamiltonian for the i-th one electron D^0 system and V_{ee} is the electron-electron repulsive Coulomb interaction. Using cylindrical coordinates and the effective Bohr radius, $a_B = \hbar^2\epsilon_0/m^*e^2$, and the effective Rydberg, $R_y = e^2/2\epsilon a_B$, as units of length and energy respectively, the neutral donor Hamiltonian $H_i^{D^0}$ and the electron-electron Coulomb potential assume the form

$$H_i^{D^0} = -\nabla^2 + \frac{\gamma}{i}\frac{\partial}{\partial\phi_i} + \frac{1}{4}\gamma^2\rho_i^2 - \frac{2}{|\vec{r}_i - \zeta|} + V_{QW}(z), \tag{2}$$

$$V_{ee}(|\vec{r}_1 - \vec{r}_2|) = \frac{2}{|\vec{r}_1 - \vec{r}_2|}, \tag{3}$$

where the vector potential is taken in the symmetric gauge $\vec{A} = \vec{r}\times\vec{B}/2$. The magnetic field is expressed in the dimensionless quantity $\gamma = \hbar\omega_c/2R_y$ with $\omega_c = eB/m^*c$ the cyclotron frequency; ζ is the position of the donor along the z-axis as measured from the center of the well and $V_{QW}(z)$ is the confining potential due to the quantum well of width W. For $GaAs/Al_xGa_{1-x}As$ with $x = 0.25$ we took $\epsilon = 12.5$ and obtain $a_B = 98.7$Å, $R_y = 5.83\ meV$, $\gamma = 0.148B(T)$. We took the mass of the electron equal in the well and in the barrier, namely $m^* = 0.067m_0$, and the height of the barrier is given by $V_0 = 0.6\times(1.155x + 0.37x^2)\ eV$.

The strong confinement along the z-axis allows to neglect the correlation induced by the Coulomb interaction in the z-direction, thus we can write the wave functions for the D^- as follows

$$\Psi(\vec{r}_1,\vec{r}_2)=\psi(\vec{\rho_1},\vec{\rho_2})f_1(z_1)f_1(z_2), \tag{4}$$

with $f_1(z_i)$ the 1D ground state wave function for the electron confined in a quantum well of height V_0.[10]

The two-electron function $\psi(\vec{\rho_1},\vec{\rho_2})$ expresses the correlation between the two electrons and is obtained by diagonalizing the Hamiltonian (1) in which the electron-electron, V_{ee}, and the electron-donor, V_{ed}, Coulomb interaction are replaced by their average along the z-axis,

$$V_{ee}(|\vec{\rho}_1-\vec{\rho}_2|)=\int dz_1\int dz_2|f_1(z_1)|^2|f_1(z_2)|^2\frac{2}{\sqrt{(\vec{\rho}_1-\vec{\rho}_2)^2-(z_1-z_2)^2}}, \tag{5}$$

and

$$V_{ed}(\vec{\rho})=\int dz|f_1(z)|^2\frac{2}{\sqrt{\rho^2+(z-\zeta)^2}}, \tag{6}$$

respectively. In a previous work[9] it has been shown that in the case of hard wall confinement Eq. (5) can be replaced by the expression

$$V_{ee}(|\vec{\rho}_1-\vec{\rho}_2|)=\frac{2}{\sqrt{2\pi}\lambda}e^{|\vec{\rho}_1-\vec{\rho}_2|^2/4\lambda^2}K_0(\frac{|\vec{\rho}_1-\vec{\rho}_2|^2}{4\lambda^2}), \tag{7}$$

where $\lambda\cong 0.2W$ and $K_0(x)$ is the modified Bessel function of the third kind. In the present paper we use the same expression for a finite height quantum well in which λ is determined by fitting Eq. (7) to Eq. (5). A comparison between the potential (5) that was evaluated numerically and the approximate expression (7) is shown in Fig. 1(a) for a quantum well of width $W=200$Å where the fitting parameter was found to be $\lambda=0.607a_B$. On the other hand, no simple analytic approximation to Eq. (6) could be found. This is shown in Fig. 1(b) for an off-center donor with $\zeta=0.7a_B$ and $W=200$Å where we compare Eq. (6) which we fitted to the potential (7) with $\lambda=0.92a_B$ (solid curve) and the screened Coulomb potential $1/\sqrt{\rho^2+\lambda^2}$ with $\lambda=0.803a_B$ (dashed curve). None of the two fits give a good approximation to Eq. (6) in the small ρ region. Therefore, we retain in the Hamiltonian the numerical expression for Eq. (6).

Using a finite difference technique, as explained in Ref. 12, the Schrödinger equation associated to the Hamiltonian (2) was numerically solved on a non-uniform grid in $\vec{\rho}$-space and the eigenvalues and eigenvectors, $R_{n,l}(\rho)e^{il\phi}$ for the D^0 were found for different values of ζ and arbitrary magnetic field strength. The eigenfunctions for the D^- can then be constructed as a linear combination of the D^0 wave functions. Due to the rotational symmetry in the $\vec{\rho}$-plane of the Hamiltonian (2) the z-component of the orbital angular momentum, L, is a good quantum number for those functions, and therefore the D^- wave functions are taken as

$$\psi_L(\vec{\rho}_1,\vec{\rho}_2)=\sum_{k=1}^{k=k_m}\sum_{n=1}^{n=n_m}\sum_{l=-l_m}^{l=l_m}{}'\,C^l_{kn}R_{n,(L+l)/2}(\rho_1)R_{k,(L-l)/2}(\rho_2)e^{i[l(\phi_1$$

(8)

where $\sum'$ indicates the summation is only over even (odd) values of the index l when L is even (odd).

III. THE ENERGY SPECTRUM

First we solve our model for an off-center donor in a ~~GaAs/Al~~$Ga_{.7}As$ quantum well with width $W=200$Å ($\approx 2a_B^*$) and height of the potential barrier $V_0=0.23eV$. The dependence of the energy on the position of the donor with respect to the center of the well is investigated numerically.

The binding energy of the D^- state with $\hat{z}$-component of the orbital angular momentum equal to L is defined as

$$E_b^n(D^-,L)=E^0(D^0,0)+E(e,0)-E^n(D^-,L), \tag{9}$$

where $E^0(D^0,0)$ is the energy of the ground state of the D^0 in the well, $E(e,0)=\gamma$ is the energy of a free electron in the $N=0$ Landau level and $E^n(D^-,L)$ is the n-th energy level of the D^- with L the $\hat{z}$-component of the orbital angular momentum.

The results of our numerical calculation are plotted in Fig. 2 for $W=200$Å. The binding energies of the first L=0 state, a spin-singlet, and of the state L=-1, a spin-triplet, are plotted against the magnetic field for different positions, ζ, of the donor with respect to the center of the well.

We note, first, that the binding energy decreases when the donor center is displaced from the center of the quantum well. The reason is that the electron-donor interaction decreases with increasing ζ. This is because, due to the strong confinement along the growth axis of the well, the electrons tend, even in the case of an off-center donor system, to be localized in the center of the quantum well although the donor is displaced a distance ζ from the center.

A second feature to be noted is that the magnetic field dependence of the binding energy changes qualitatively with increasing ζ. For sufficiently large ζ we find that $E_b^n(D^-,L)$ has a maximum as function of γ. The binding energy starts to decrease after this maximum and for sufficiently large γ it can even become negative, indicating an unbinding of the D^- state.

Third, in the absence of a magnetic field the ground state of the D^- is, regardless of the position of the donor, the spin-singlet state. When increasing the magnetic field, the ground state for a well-center D^-, i.e. $\zeta=0$, remains the singlet one. In contrast, the ground state of the off-center D^- with $\zeta>.45a_B$ shows a transition to

a spin-triplet state for large enough magnetic fields. The magnetic field at which the singlet-triplet transition occurs depends on the position of the donor as it appears from Fig. 2. This dependence will be studied further below where it is found that the magnetic field at which the transition occurs decreases with increasing ζ.

Larsen and coworkers[6] investigated the ideal 2D problem, neglecting the finite extension of the electron wave function in the z-direction, i.e. $f_1(z) = \delta(z)$, and calculated the D^- spectrum for a donor out of the plane in the limit of high magnetic fields and found an infinite number of singlet-triplet transitions. The situation for a quasi-2D off-center D^- is quite different. In this case, in contrast to the 2D case, the extension of the electron wave function in the z-direction is taken into account, together with the finite height of the barrier. Let us investigate deeper the behavior of the energy spectrum of such a system, with e.g. $\zeta = 0.7a_B$. The results for the binding energy of the different levels, i.e. different angular momentum states, are shown in Fig. 3(a), for the case of a quantum well of width $W = 200$Å. Note that different transitions occur at higher magnetic fields. The ground state exhibits a singlet-triplet transition at $\gamma = 1.5$ and a triplet-singlet transition at $\gamma = 16.1$. For $\gamma > 22.7$ which corresponds to $B > 154\,T$ the D^- ground state unbinds, i.e. the D^- *magnetically evaporates*.

While for the ideal 2D system an infinite number of singlet-triplet transitions are found for a quasi-2D system only a finite number of such transitions are possible as is clearly visible from Fig. 3(a,b). The critical γ's at which the singlet $\leftrightarrow$ triplet transitions occur depend on the position of the donor (see Fig. 3(b)). The $\gamma - \zeta$ phase diagram for the ground state of a quantum well of width $W = 200$Å is given in Fig. 4. We found that for $\zeta < 0.45a_B$ the ground state is a singlet for all magnetic fields, for $0.45a_B < \zeta < 0.65a_B$ only one singlet-triplet transition (see Fig. 4) is possible and for $\zeta > 0.65a_B$ there are two of such transitions. Increasing ζ further such that the donor is in the barrier (i.e. $\zeta > 1.01a_B$), the number of singlet-triplet transition does not increase as illustrated in Fig. 3(b) for a D^- with $\zeta = 1.4a_B$.

The physical origin of the singlet-triplet transitions is related to the decrease of the electron-donor attraction with the displacement of the donor from the center of the well when compared to the constant electron-electron repulsion. The corresponding electron-donor and electron-electron in-plane potentials are shown in Fig. 5 for two values of ζ. For small values of ζ (e.g. $\zeta = 0.$ in Fig. 5) the attractive single electron-donor potential is larger than the electron-electron potential and consequently the D^- system prefers a configuration in which the two electrons are as close as possible to the donor in order to enhance the binding energy, i.e. the L=0 state is favored. When ζ is sufficiently large (e.g. $\zeta = 0.7a_B$ in Fig. 5) the repulsive electron-electron interaction dominates the attractive single-donor potential at small distances and the D^- can have bound states only when the two electrons are sufficiently apart to render the repulsive inter-electrons interaction lower or of the same order as the attractive electron-donor potential. For small magnetic fields this can still be realized in the L=0 state. Increasing the magnetic field brings the electrons closer to $\rho = 0$ which will also increase the electron-electron repulsive energy. For sufficiently small ζ this can still be compensated by the attractive electron-donor energy. For ζ sufficiently large the electron-electron repulsive energy increases faster then the electron-donor energy with increasing B. The D^- system can decrease its energy in this case by placing the electrons further apart which is achieved by placing the electrons in higher L-states. Similar singlet-triplet transitions have been found recently in quantum dots systems.[11–13] The quantum dot system is an extreme case in which the electron-donor potential is replaced by the confinement potential which is usually taken of a quadratic form, i.e. $V_{ed} \rightarrow \omega^2\rho^2$.

In Fig. 6 the pair-correlation function $< \delta(\rho - |\vec{\rho}_1 - \vec{\rho}_2|) >$ is shown for the spin-singlet L=0 (Fig. 6(a)) and spin-triplet L=-1 (Fig. 6(b)) states for different values of the magnetic field for an on-center (i.e. $\zeta = 0$) and for an off-center (i.e. $\zeta = 0.7a_B$) D^- system. The magnetic field behavior of the two states is essentially the same for both the center and the off-center D^- system. The magnetic field tends to localize more the wave function with increasing magnetic field. For the L=0 state the pair correlation function becomes more and more peaked at $\rho = 0$, this means that the electrons are more and more close to each other with increasing magnetic fields. For the L=-1, the peak of the correlation function is shifted towards $\rho = 0$ with increasing B, and thus, the magnetic field localizes the electrons further. The effect of the electron-electron repulsion can be seen in the shape of the correlation function itself. For the off-center system the pair-correlation function is broader than the one for the center D^- system even for increasing magnetic fields and thus the electrons tend to repel each other more, which is a consequence of the diminished electron-donor interaction.

When the dimension of the well is reduced the localization of the electrons in the center of the well is increased. For example, if we neglect the penetration of the electrons in the barrier, the width of the $f_1(z)$ is equal to L. Thus the electron-electron repulsion increases and at the same time, for the off-center case, the electron spends more time far from the position where the donor is located. Thus, we expect that systems with a smaller well width will show more spin-singlet to spin-triplet transitions with increasing magnetic field, and that these transitions will occur at smaller fields.

Indeed, for a $W = 100$Å quantum well, with again $\zeta = 0.7a_B$, we observe (see Fig. 7) as much as 4 transitions before the D^- evaporates at a magnetic field of $B \approx 81T$ (i.e. $\gamma \approx 12.0$). The full phase-diagram for those transitions is shown in Fig. 8. The well width dependence of the singlet-triplet transitions and of the evaporation magnetic field are shown in Fig. 9 for $\zeta = 0.7a_B$. Notice that the critical magnetic field for the

same transitions, e.g. for the spin-singlet L=0 to spin-triplet L=-1 state, decreases with decreasing well width. At the same time the number of transitions increases. But the evaporation magnetic field first decreases and then for $W < 140$Å increases again. An explanation of this feature is that other transitions are allowed for small well width and this ensure stability of the D^- up to higher magnetic fields.

The increase of the number of singlet-triplet transitions with decreasing dimensions of the quantum well, explains the larger number of transitions found by Larsen *et al.*[6] in the ideal 2D system with respect to the smaller number found in the present study of realistic quasi-2D systems.

IV. CYCLOTRON RESONANCE TRANSITIONS

The oscillator strength for cyclotron transitions, in the present units, is defined as

$$F_{i,f} = (E_f - E_i)| < \Psi_i| \sum_{j=1}^{2} \frac{1}{2} \rho_j e^{\pm i\phi_j} |\Psi_f > |^2 \qquad (10)$$

where E_f, E_i are, respectively, the final and initial-state energies and ψ_f, ψ_i are, respectively, the final and initial-state wave functions. The $\pm$ sign in Eq. (10) refers to circular left/right polarization of the light. Note that the perturbation induced by the electric field is spin-independent, thus the initial and final-states conserve the total spin, i.e. they are both spin-triplet or both spin-singlet states. Eq. (10) leads to the selection rules $\Delta L = \pm 1$, while no selection rule is present for the quantum number n.

We have studied the oscillator strength for cyclotron resonance transitions from the first singlet L=0 state - (n,L,S)=(1,0,0) - to the (1,-1,0) and the (1,1,0) states in the range 2-15T. The transition energies and oscillator strengths, for $\zeta = 0.7a_B$, are plotted in Fig. 10 against the magnetic field and are compared to the one for $\zeta = 0$. We recall that for a two-electron atom the oscillator strength satisfies the sum-rule $\sum_i F_{i,f} = 2$. We observe that the off-center and the center D^- have rather similar qualitative magnetic field dependences.

Cyclotron resonance transition from the ground state should show a discontinuous behavior in the cyclotron transition energies as a function of the magnetic field at the singlet-triplet transition points. In Fig. 11 the transition energies for a donor at position $\zeta = 0.85a_B$ are shown. Respectively, the transition energies for $(1,0,0) \rightarrow (1,1,0)$ and $(1,-1,1) \rightarrow (1,0,1)$ and $(1,-2,0) \rightarrow (1,-1,0)$ are plotted. The solid curve shows the transition energy which we expect to observe if the system makes a cyclotron resonance transition starting from the ground state. Thus steps in the cyclotron resonance energy should be observed at those magnetic fields at which the singlet-triplet transition takes place. In real experiments, as we will see later, not always transitions only from the ground state are seen in the neighborhood of the critical field which is due to the fact that in a real experiment the temperature is non zero. Indeed, when the *old* ground-state, i.e. the state that was before the transition the ground-state, and the *new* ground-state, i.e. the state that is after the transition the ground-state, have a comparable binding energy they can both be thermally populated.

V. COMPARISON WITH EXPERIMENT

In this section we present a comparison between our theoretical results and the experimental data reported by Jiang *et al.*[8] The experiment of Jiang *et al.* was performed on multi-layers of $GaAs/Al_{.3}Ga_{.7}As$ with well width of 200Å and barrier width of 600Å. Such a system can be considered as an ensemble of single quantum wells. The wells were nominally δ-doped at 3/4 of the distance between the center of the well and its edge. In the model discussed in this paper this means that $\zeta = .75a_B$.

A comparison between the theoretical and the experimental transition energies is reported in Fig. 12. The observed transitions are the D^0 $(1,0) \rightarrow (1,1)$ and the D^- singlet $(1,0,0) \rightarrow (1,1,0)$ and triplet $(1,-1,1) \rightarrow (1,0,1)$ transitions. Our theoretical results are given by the three different curves. Note that our results fit well the data at low magnetic fields. The deviations between theory and experiment observed for $B > 9T$ can be attributed to band non-parabolicity and polaron effects. Both effects decrease the transition energy[2] but are not taken in account in this paper.

In cyclotron resonance experiments the integrated absorption intensities can be measured. The integrated absorption intensities are proportional to the oscillator strength times the population densities of the levels involved in the transition. To compare our results with the experimental data we have to make an assumption on the form of the population density. We assume that only the initial level of the transition is populated. Thus for the off-center D^- the population density of the level is proportional to $e^{E_b/kT}$, where E_b is the binding energy of the initial state. We remark that for off center D^- in this range of magnetic fields the energies of the triplet and the singlet states are comparable. For the well-center D^-, instead, we consider only the L=0 spin-singlet state to be populated, i.e. the population density is 1.

The results for the relative integrated intensities of the singlet transition as evaluated in our calculation and the experimental results are plotted in Fig. 13 and are in good agreement, both for the well-center as well as for the off-center D^-. The temperature in the experiment was $T = 4.3K$. Note that the different magnetic field dependence for the center D^- (i.e. increase with B) and for the off-center D^- (i.e. decrease with B) is correctly described. The errors bars for the off-center intensities

are rather large. A slight discrepancy is observed at certain values of the magnetic field for the off-center D^- but we observe that moving the donor in our model slightly closer to the center of the well, i.e. $\zeta = 0.7a_B$, the relative integrated intensity changes from the solid to the dotted curve in Fig. 13 and now matches the experimental data in the magnetic fields region in which there was not such a good agreement before. Thus the apparent discrepancy in the integrated intensity, with $\zeta = 0.75a_B$, in the range $5 - 14\ T$ is explained by considering a small distribution of donors around the point of intended δ-doping.

VI. SUMMARY AND CONCLUSION

We presented a theoretical study of the off-center D^-, where special attention was paid to the dependence of the binding energy on the well width and the donor position. We found that the magnetic field induces spin-singlet to spin-triplet transitions in the ground-state of the off-center D^-. The number of those transitions depends *both* on the position of the donor and on the width of the well. In contrast to the ideal 2D system and to quantum dots only a finite number of transitions are found. If the donor is near the center of the quantum well no such singlet-triplet transitions occur. When such singlet-triplet transitions occur we find that at sufficiently large magnetic field the D^- system becomes unbound and consequently one observes a magnetic evaporation of the D^- system. We calculated also the oscillator strength for the off-center D^- as function of the magnetic field and compared it to the results for a center D^-. We restrain ourselves to the study of the optical transitions $(1,0,0) \rightarrow (1,-1,0)$, $(1,0,0) \rightarrow (1,1,0)$, and we observed that the off-center and the center D^- have similar magnetic behaviour. Our results were used to explain the experimental results recently reported by Jiang *et al.* on the cyclotron resonance transition energy and the absorption intensity of the off-center D^- system for magnetic fields up to $15T$.

In conclusion, the D^- center is a natural quantum dot system which is confined by the coulomb potential of the impurity and consequently is more closely related to real atomic systems. A remarkable feature of the D^- centers in quantum wells is the controllability of the effective confinement potential which is Platzmann-like for a donor in the center of the well and screened Coulomb-like when the donor is placed far away from the quantum well center. In the latter case the potential is parabolic near the center of the quantum well plane and thus resembles the confinement potential of quantum dots. In this case singlet-triplet transitions are found as function of the magnetic field. A crucial difference with the quantum dots is that only a finite number of such a transitions occur and that for sufficiently large magnetic fields the D^- system becomes unbound, i.e. magnetically evaporates.

VII. ACKNOWLEDGMENT

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FIG. 1. Comparison between the numerical evaluation and the analytical fitting of the average in-plane potentials for a quantum well of width $W = 200$Å. In (a) the e-e potential (5) is fitted to Eq. (7) (dashed curve). In (b) the e-d potential (6) is fitted to Eq. (7) (solid curve) and to $1/\sqrt{\rho^2 + \lambda^2}$ (dashed curve).

FIG. 2. The magnetic field dependence of the L=0 spin-singlet binding energy (solid curves) and the L=-1 spin-triplet binding energy (dotted curves) for a $GaAs/Al_{.3}Ga_{.7}As$ quantum well with width $W = 200\text{Å} = 2.02a_B$ are shown for different position, ζ, of the donor with respect to the center of the well. ζ is in units of a_B. For increasing magnetic field there is a crossing between the spin-singlet and the spin-triplet states when $\zeta > 0.45a_B$. .

FIG. 3. In (a) the binding energies for different values of the z-component of the angular momentum are shown for a D^- with the donor placed at $\zeta = .7a_b \approx 70\text{Å}$ from the center of the quantum well. In (b) the binding energies for a barrier D^- are displayed, with $\zeta = 1.4a_B \approx 140\text{Å}$.

FIG. 4. Phase diagram for a quantum well of width $W = 200$ Å. The curves show the magnetic fields at which the singlet-triplet transitions occur for given position of the donor as well as the field at which the D^- system evaporates.

FIG. 5. The in-plane electron-donor potential for the well-center D^- and for the off-center D^- are compared to the electron-electron potential.

FIG. 6. The pair correlation function of the D^-. In (a) the correlation function of the spin-singlet L=0 state is presented for different values of the magnetic field both for the off-center (dotted curves) as well as for the center D^- (solid curves). In (b) the same plot as in (a) is made but now for the spin-triplet L=-1 state.

FIG. 7. The binding energies for a D^- with $\zeta = 0.7a_B$ in a 100Å quantum well, for different values of L. Four transitions occur before the D^- system evaporates which occurs for $\gamma = 13.5$.

FIG. 8. The phase diagram for a 100Å wide quantum well. Four transitions are possible for this quantum well.

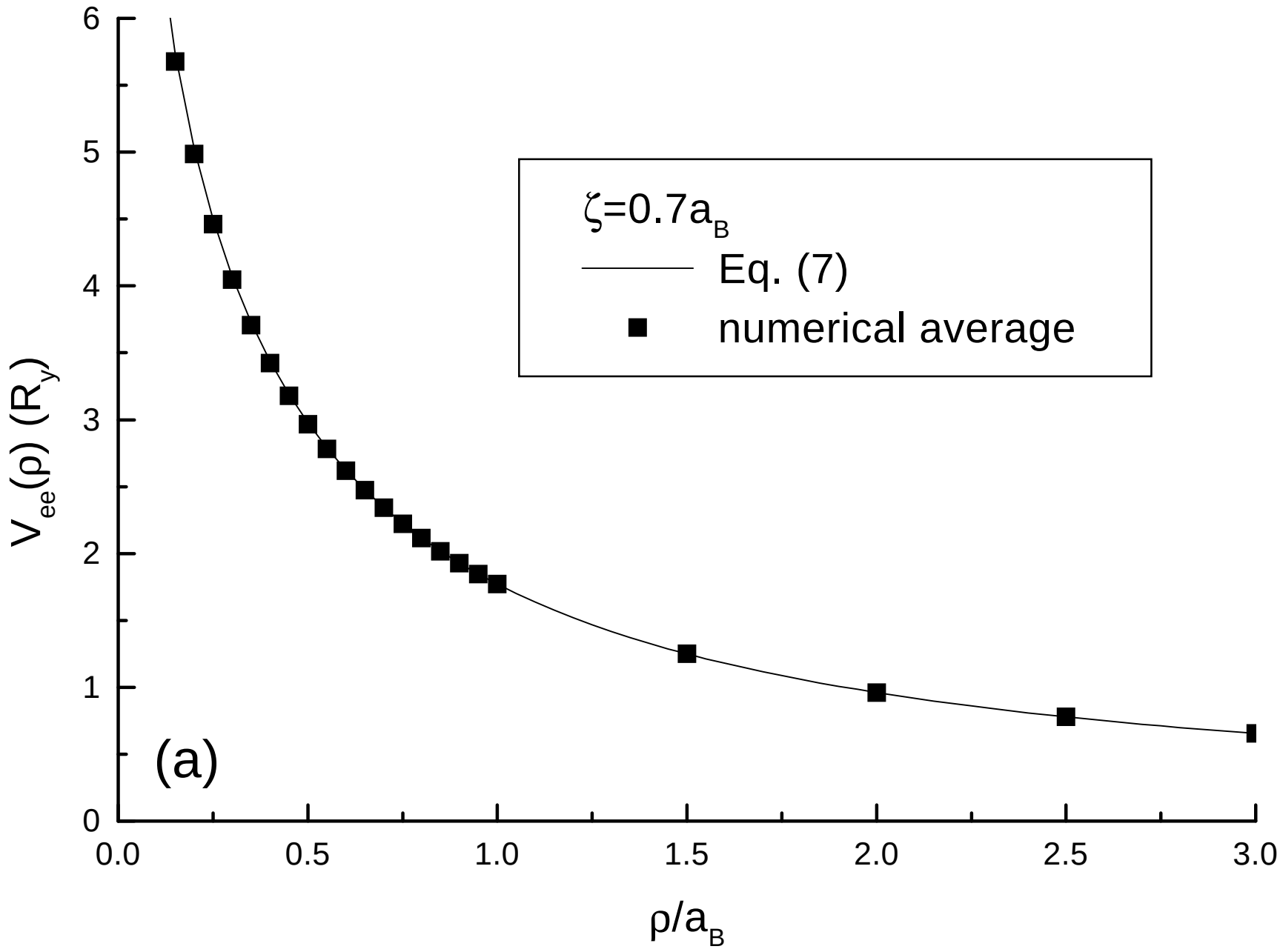
FIG. 9. The phase diagram for fixed donor position, $\zeta = 0.7a_B$, as function of the well-width W

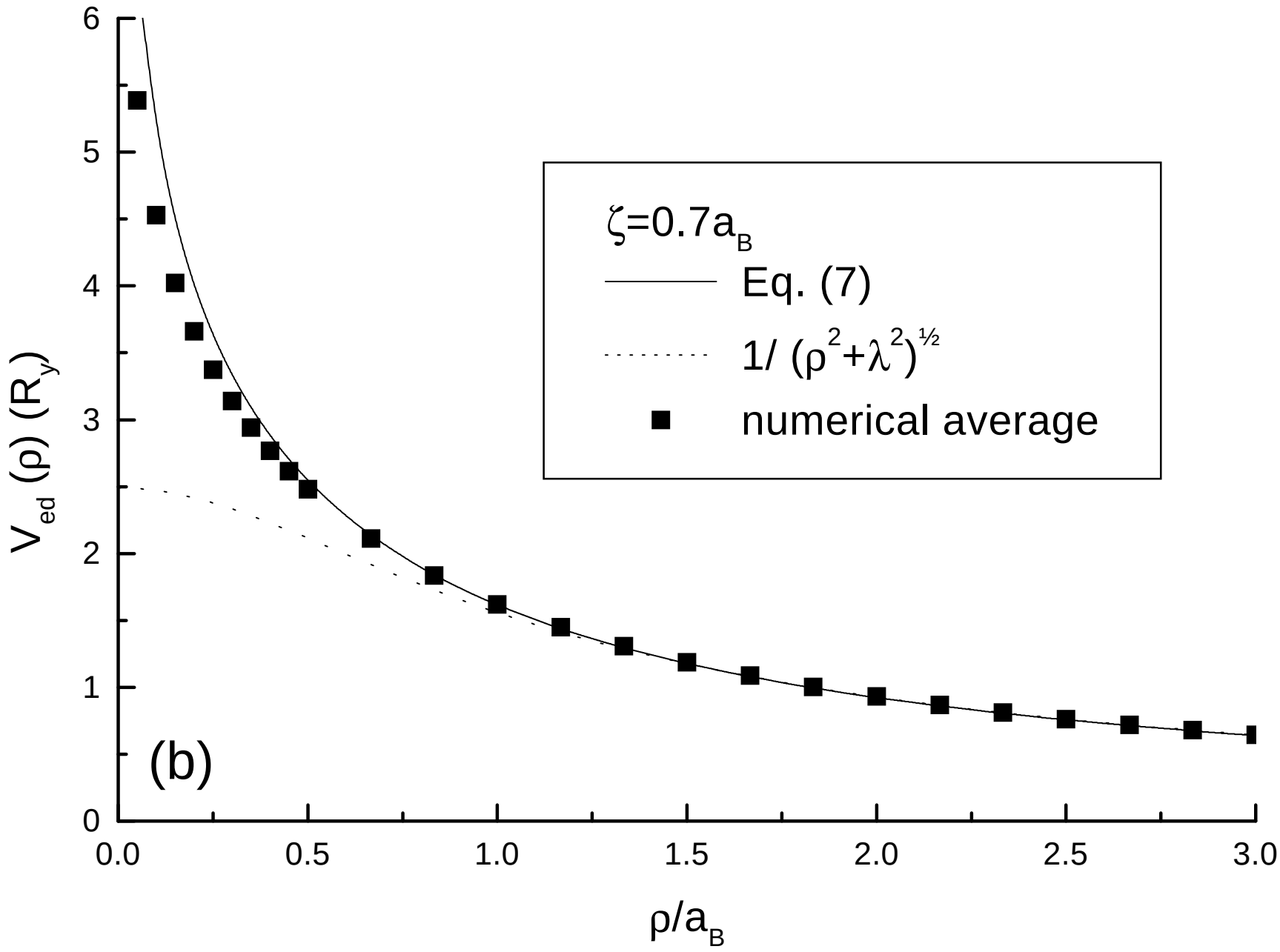
FIG. 10. The transition energies, (a), and the oscillator strengths, (b), for the $(1,0,0) \rightarrow (1,-1,0)$ and for the $(1,0,0) \rightarrow (1,1,0)$ transitions. The values for the donor placed at $\zeta = 0.7a_B$ are compared to the values for a well-center D^-. The dotted line is the free electron cyclotron transition energy, $\hbar\omega_c$.

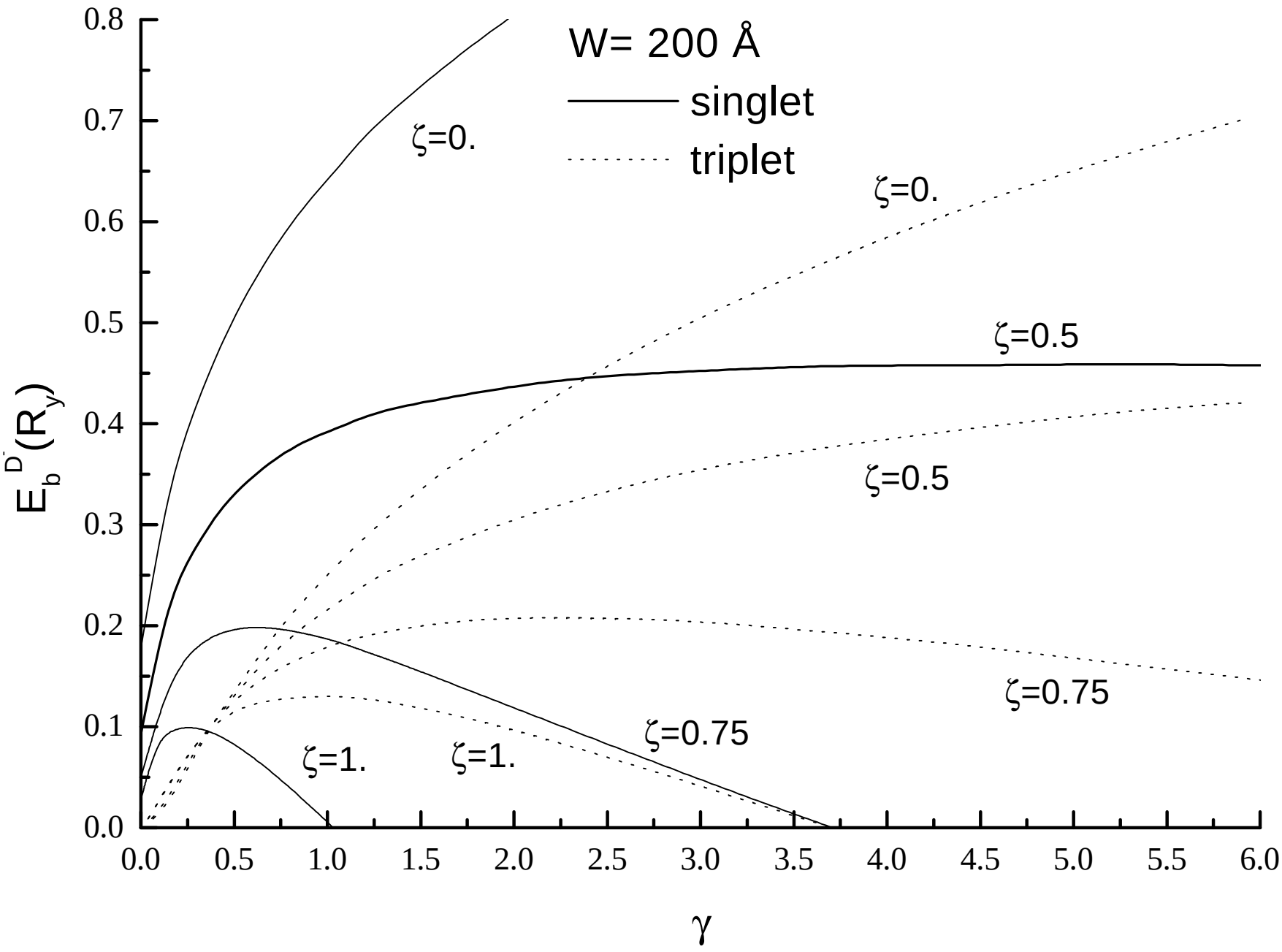
FIG. 11. The cyclotron resonance transition energies for a donor at $\zeta = 0.85a_B$ are shown by the dashed curves for the first three lowest states. The solid curve represents the expected transition energy from the ground state as function of the magnetic field at zero temperature.

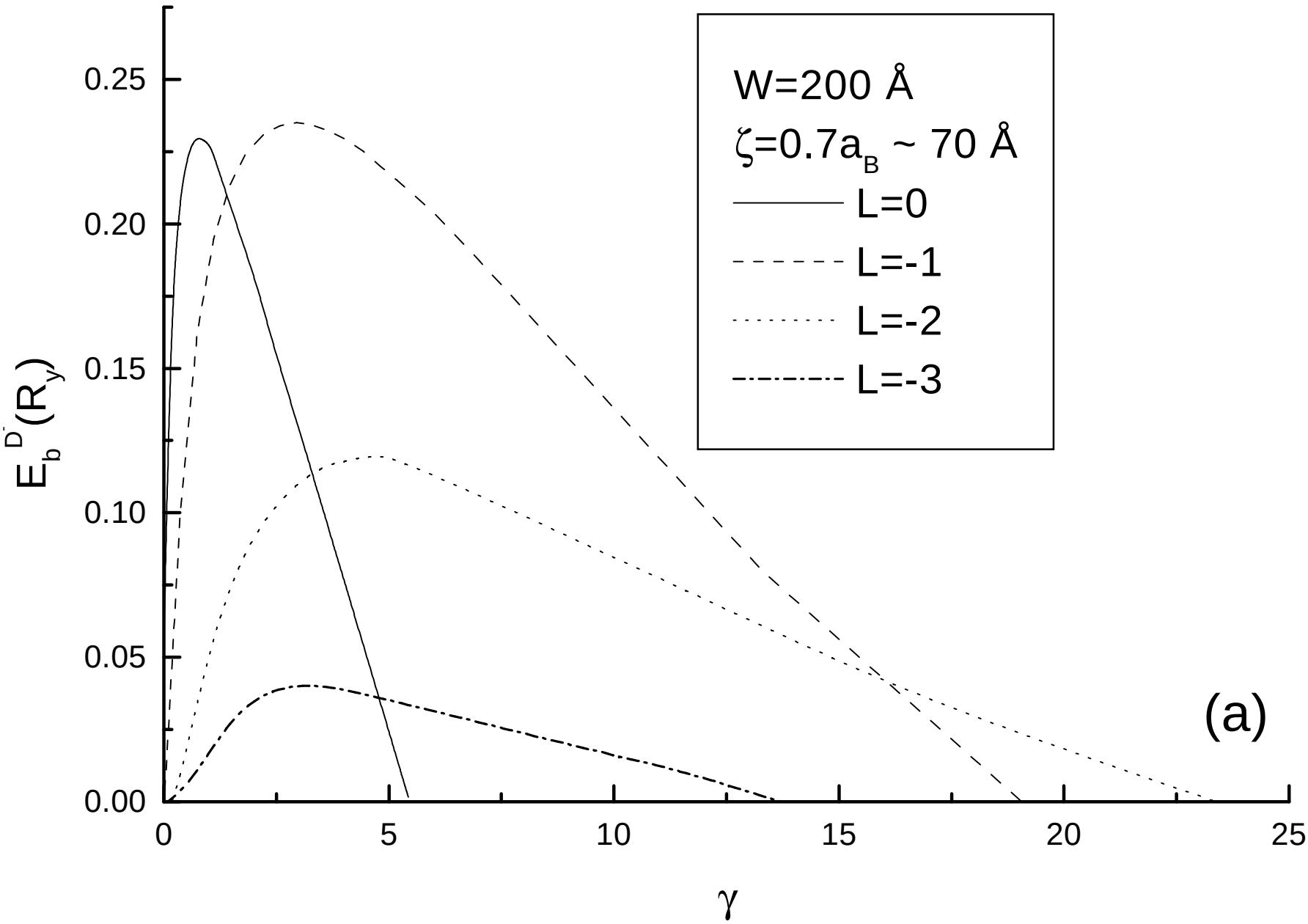
FIG. 12. The experimental data of Jiang *et al.*[8] for the cyclotron resonance transition energy (symbols) are compared to our theoretical results (curves), for the D^0 and the singlet and triplet D^-. The donor is at $\zeta = 0.75a_B$ and the well width is $W = 200\text{Å}$.

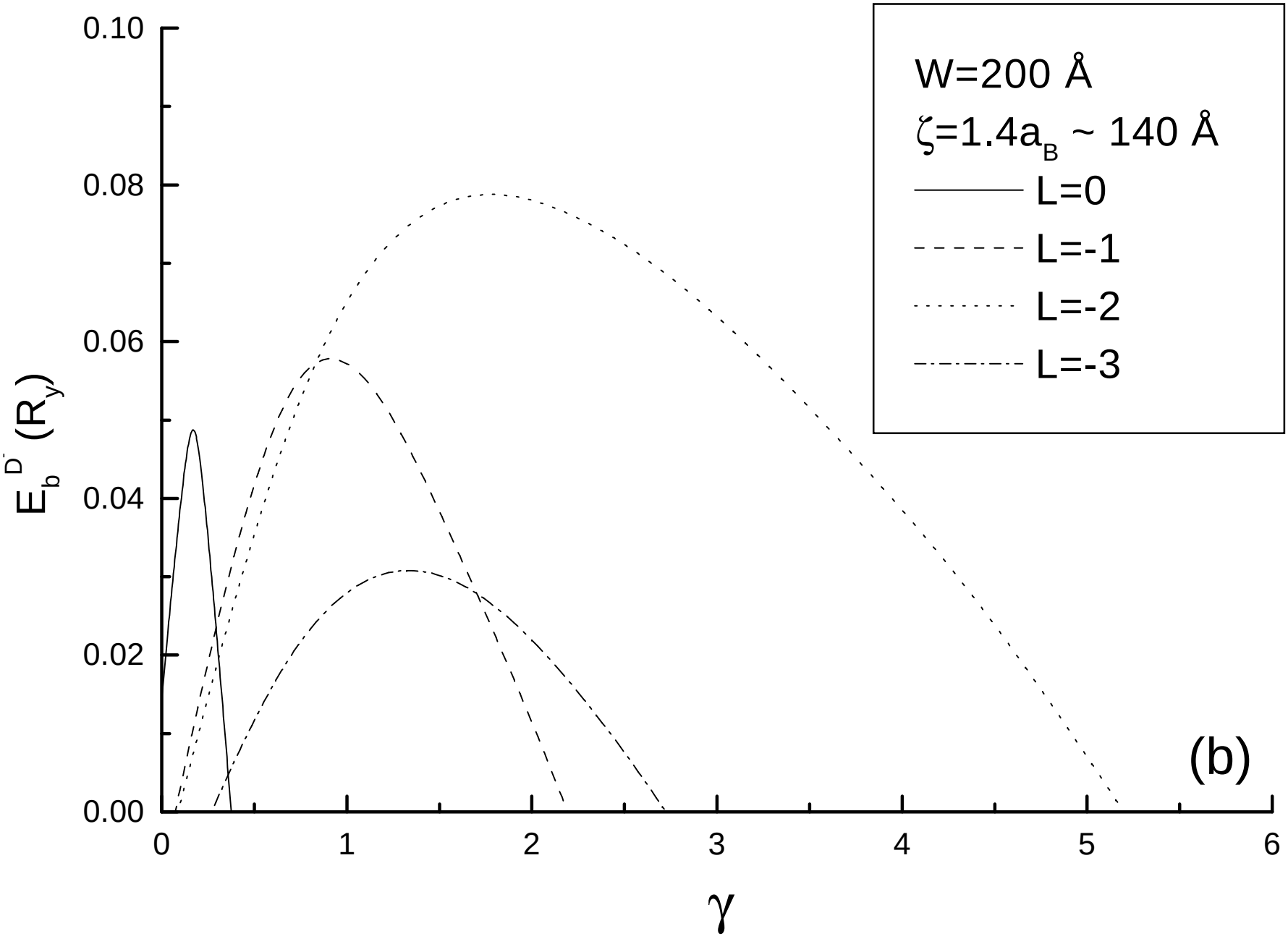
FIG. 13. Comparison of the relative integrate absorption intensity between the experimentally measured (symbols) and the present theoretical results (curves). The donor position is at $\zeta = 0.75a_B$. The dotted curve takes into account a displacement of the donor from the position at which the well is nominally δ-doped, i.e. $\zeta = 0.7a_B$.

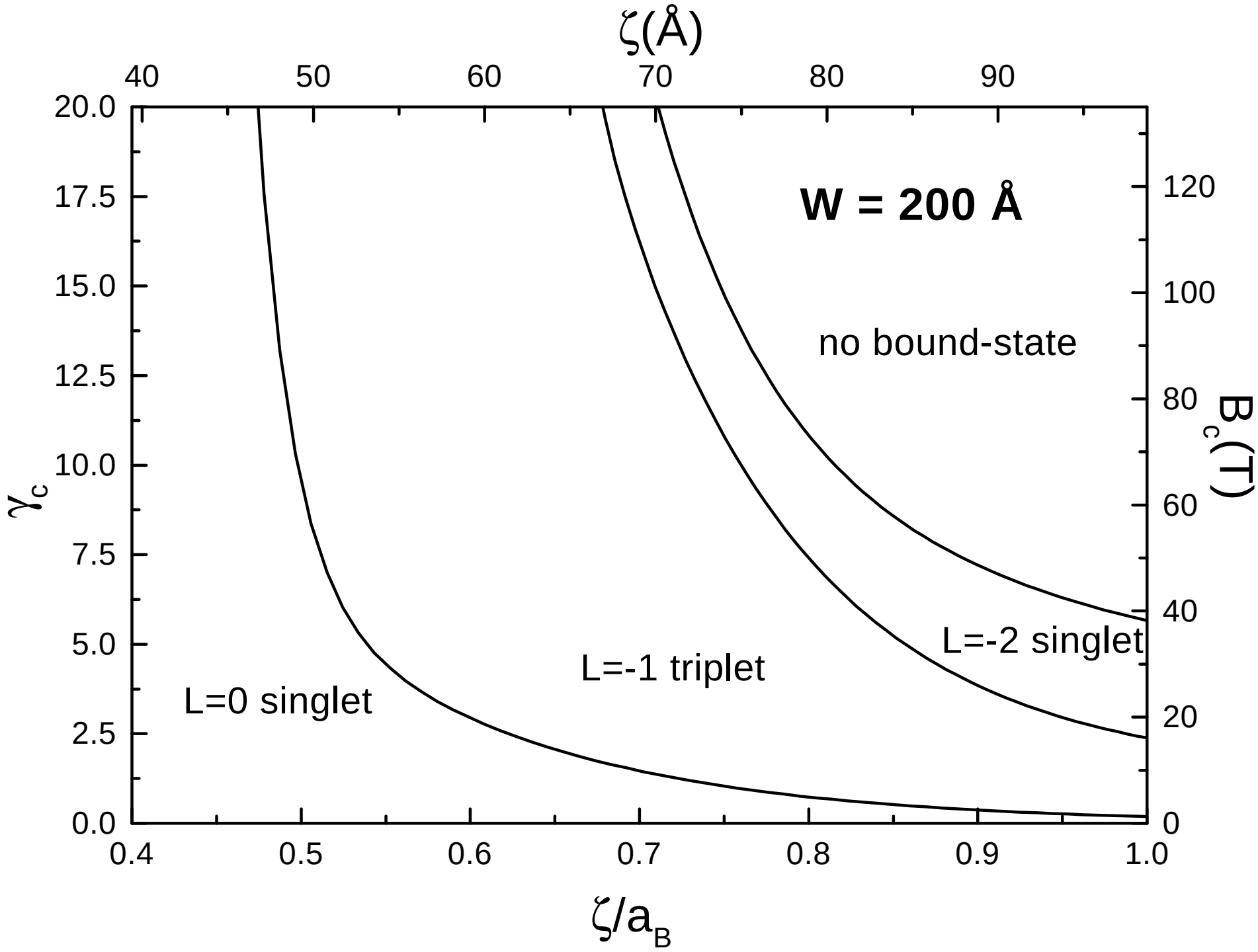

6
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
$V_{ee}(\rho)$ (R_y)
ρ/a_B
$\zeta=0.7a_B$
Eq. (7)
numerical average
(a)

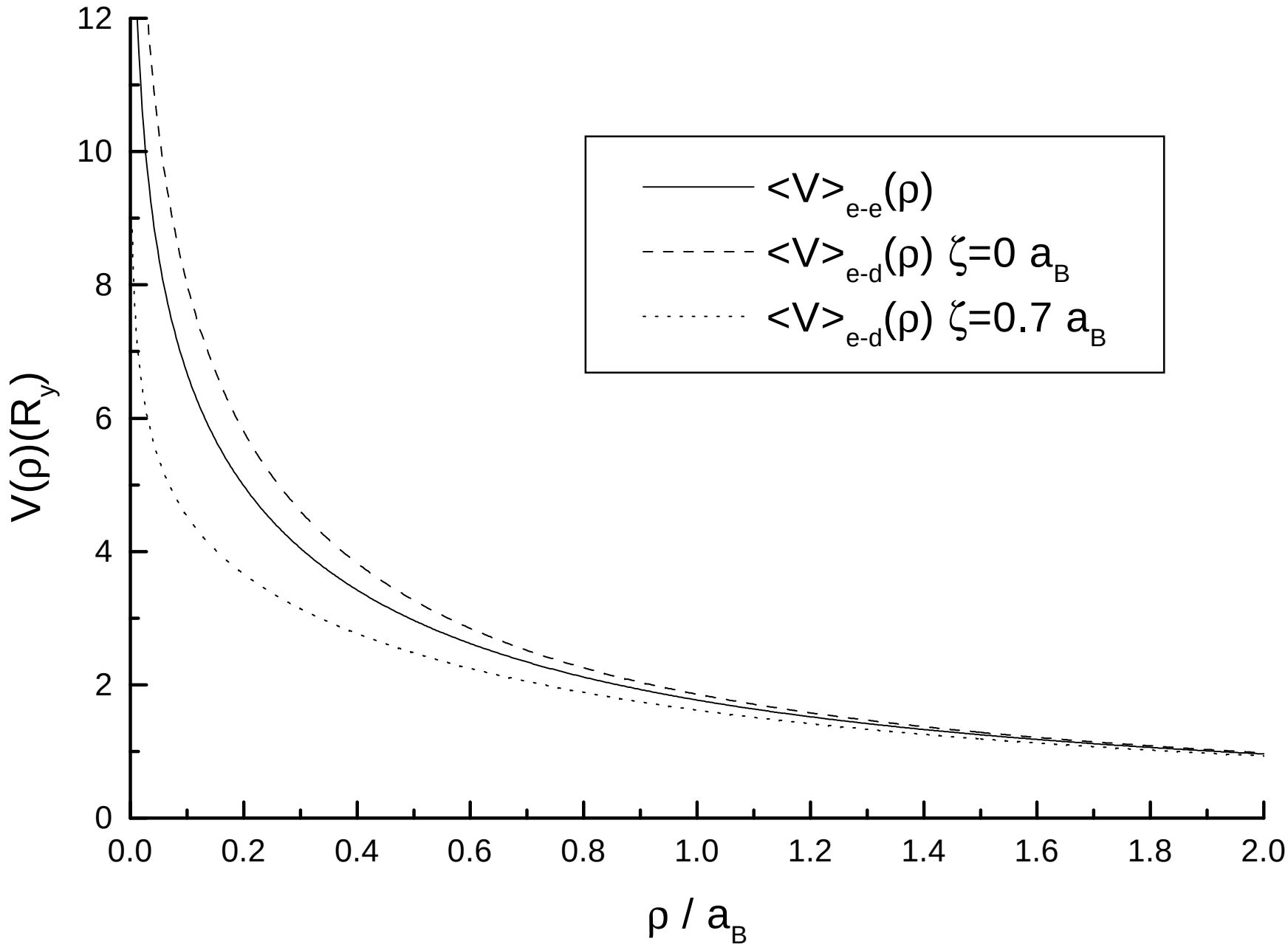

6
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
V_{ed} (ρ) (R_y)
ρ/a_B
(b)
ζ=0.7a_B
Eq. (7)
1/ ($\rho^2+\lambda^2$)^{½}
numerical average

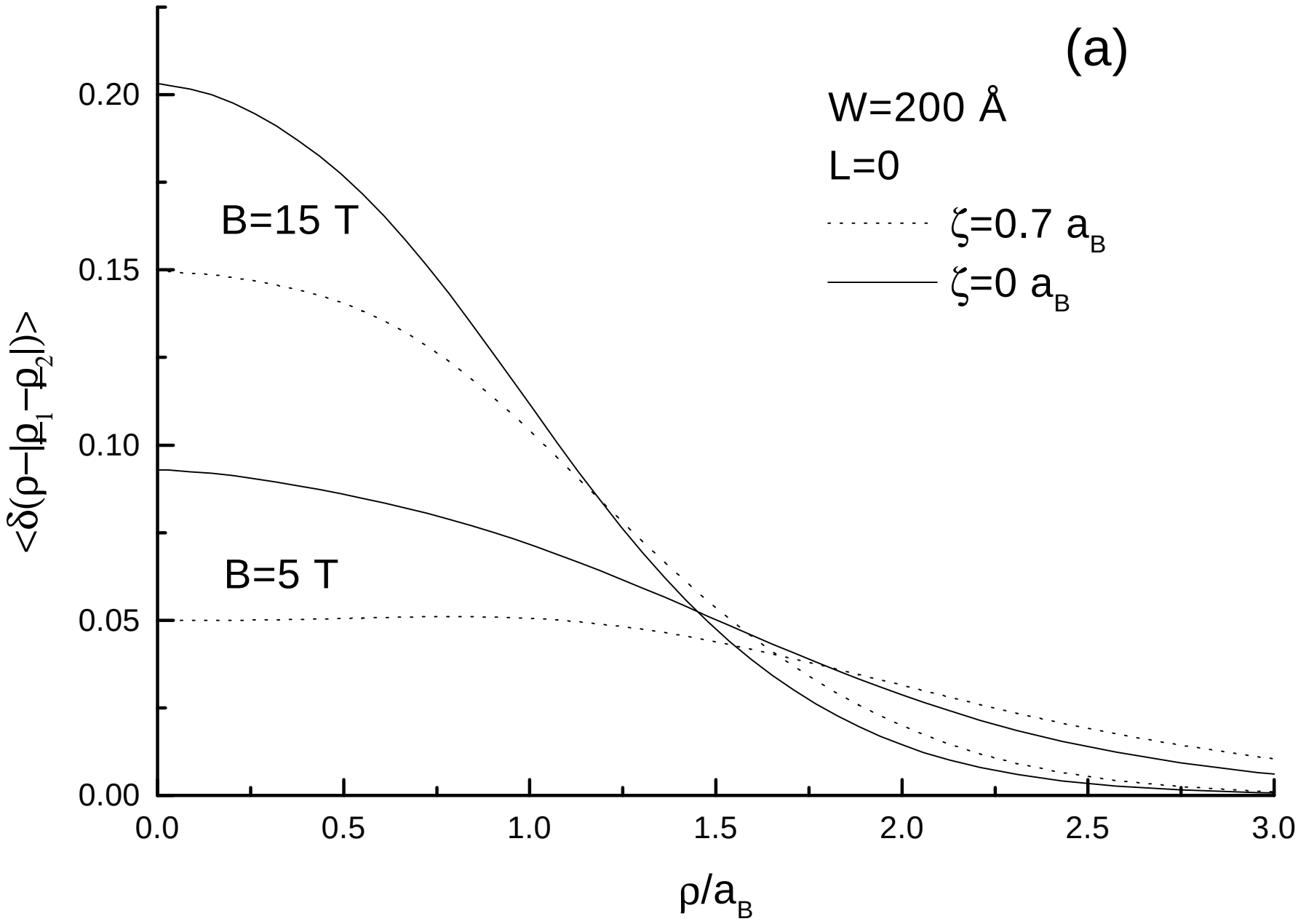

W= 200 Å
singlet
triplet
ζ=0.
ζ=0.
ζ=0.5
ζ=0.5
ζ=0.75
ζ=0.75
ζ=1.
ζ=1.
$E_b^D(R_y)$
γ
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0

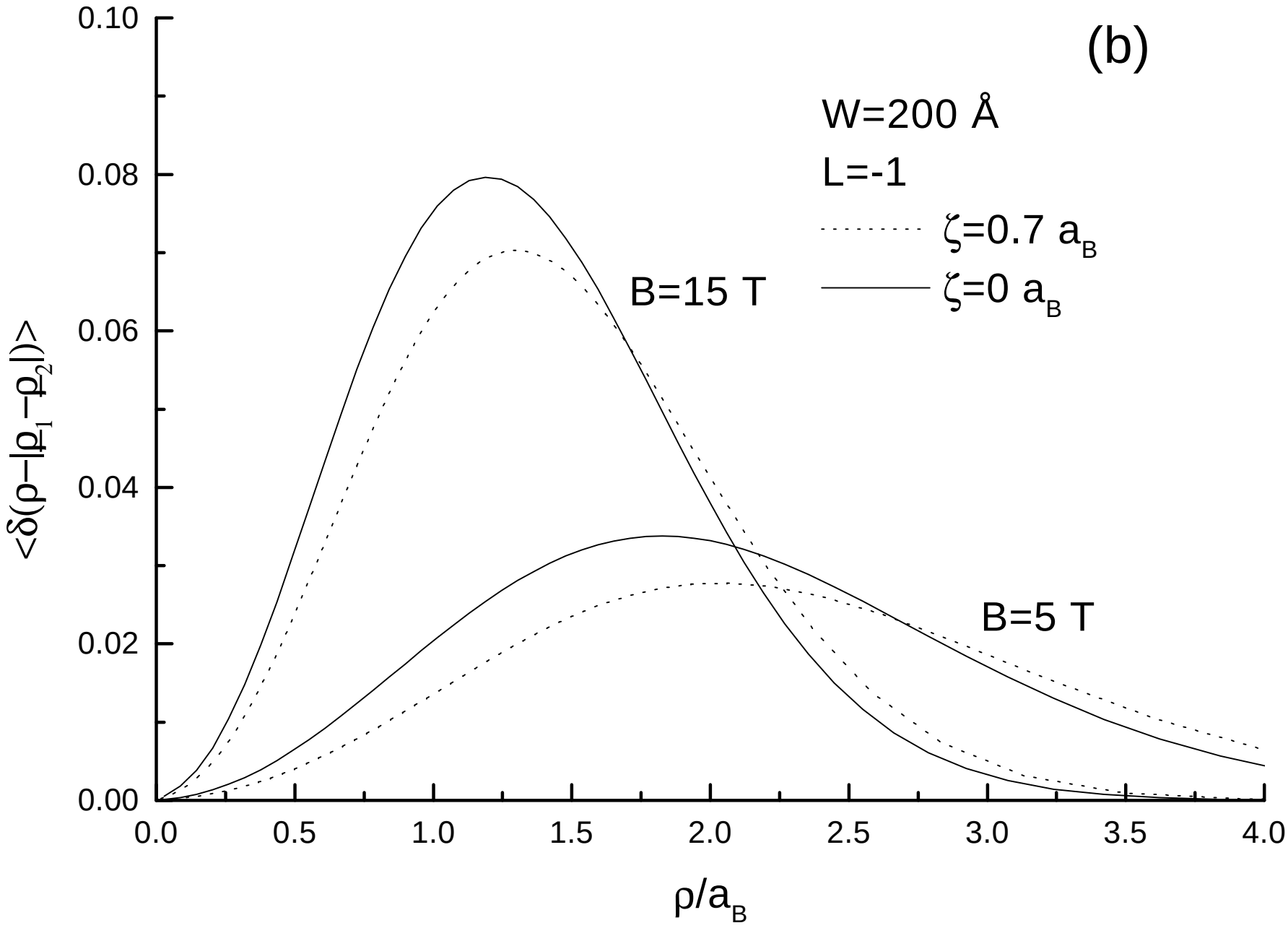

W=200 Å
ζ=0.7a_B ~ 70 Å
L=0
L=-1
L=-2
L=-3
E_b^D(R_y)
γ
(a)
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
20
25

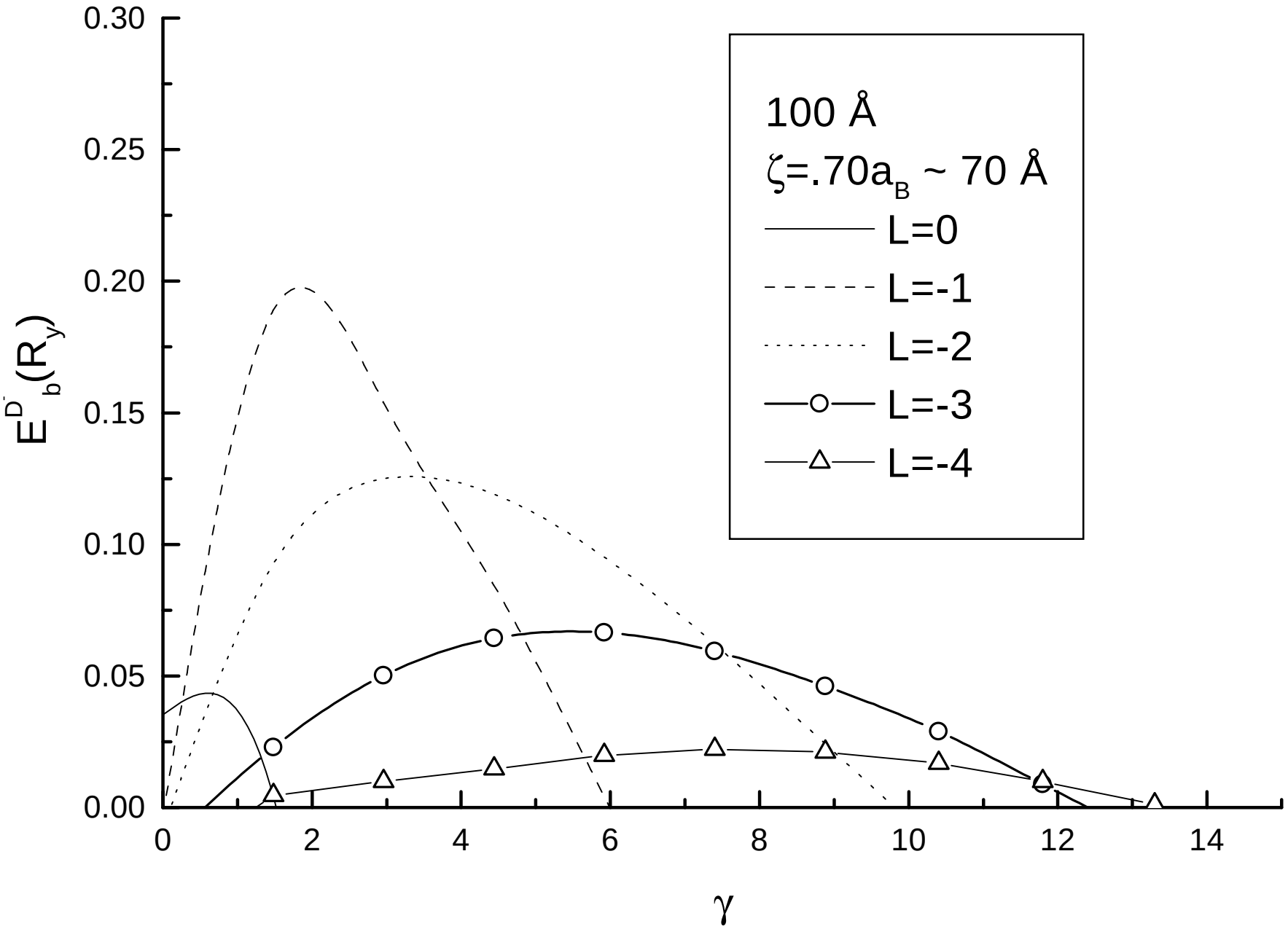

W=200 Å
ζ=1.4a_B ~ 140 Å
L=0
L=-1
L=-2
L=-3
(b)
E_b^D (R_y)
γ
0.00
0.02
0.04
0.06
0.08
0.10
0
1
2
3
4
5
6

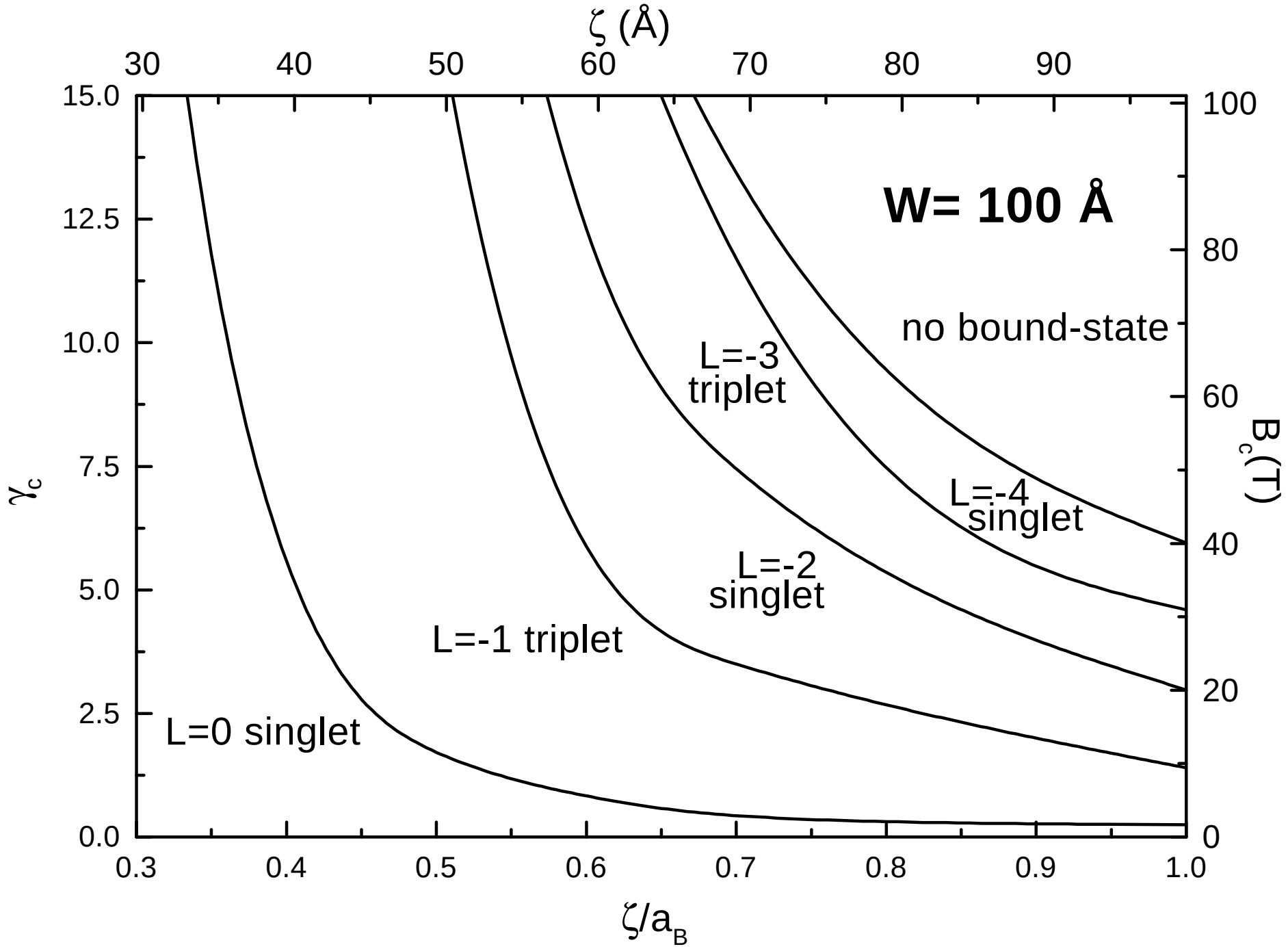

ζ(Å)
40
50
60
70
80
90
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
γc
120
100
80
60
40
20
0
Bc(T)
W = 200 Å
no bound-state
L=-2 singlet
L=-1 triplet
L=0 singlet
0.4
0.5
0.6
0.7
0.8
0.9
1.0
ζ/aB

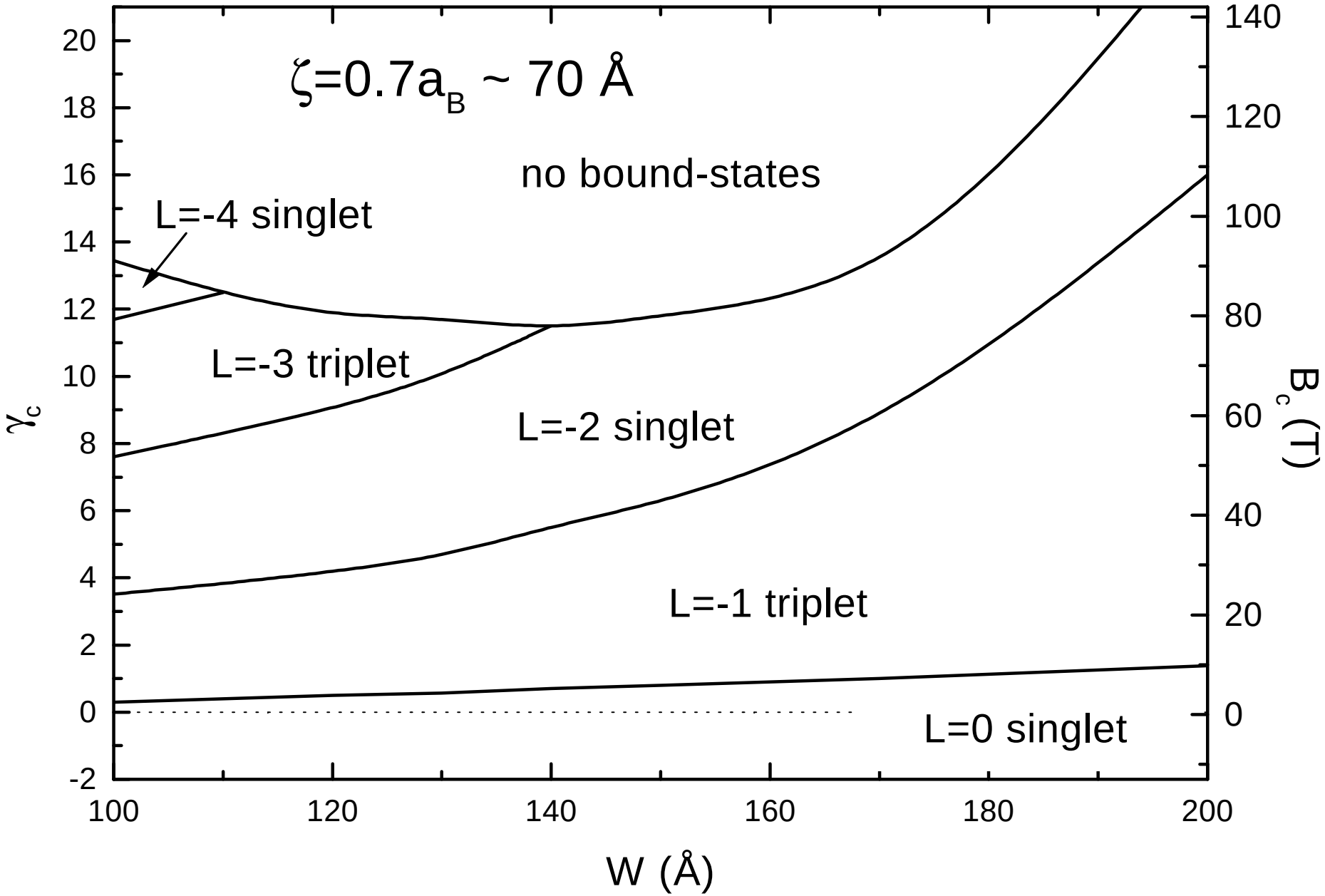

12
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
V(ρ)(R_y)
ρ / a_B
<V>_e-e(ρ)
<V>_e-d(ρ) ζ=0 a_B
<V>_e-d(ρ) ζ=0.7 a_B

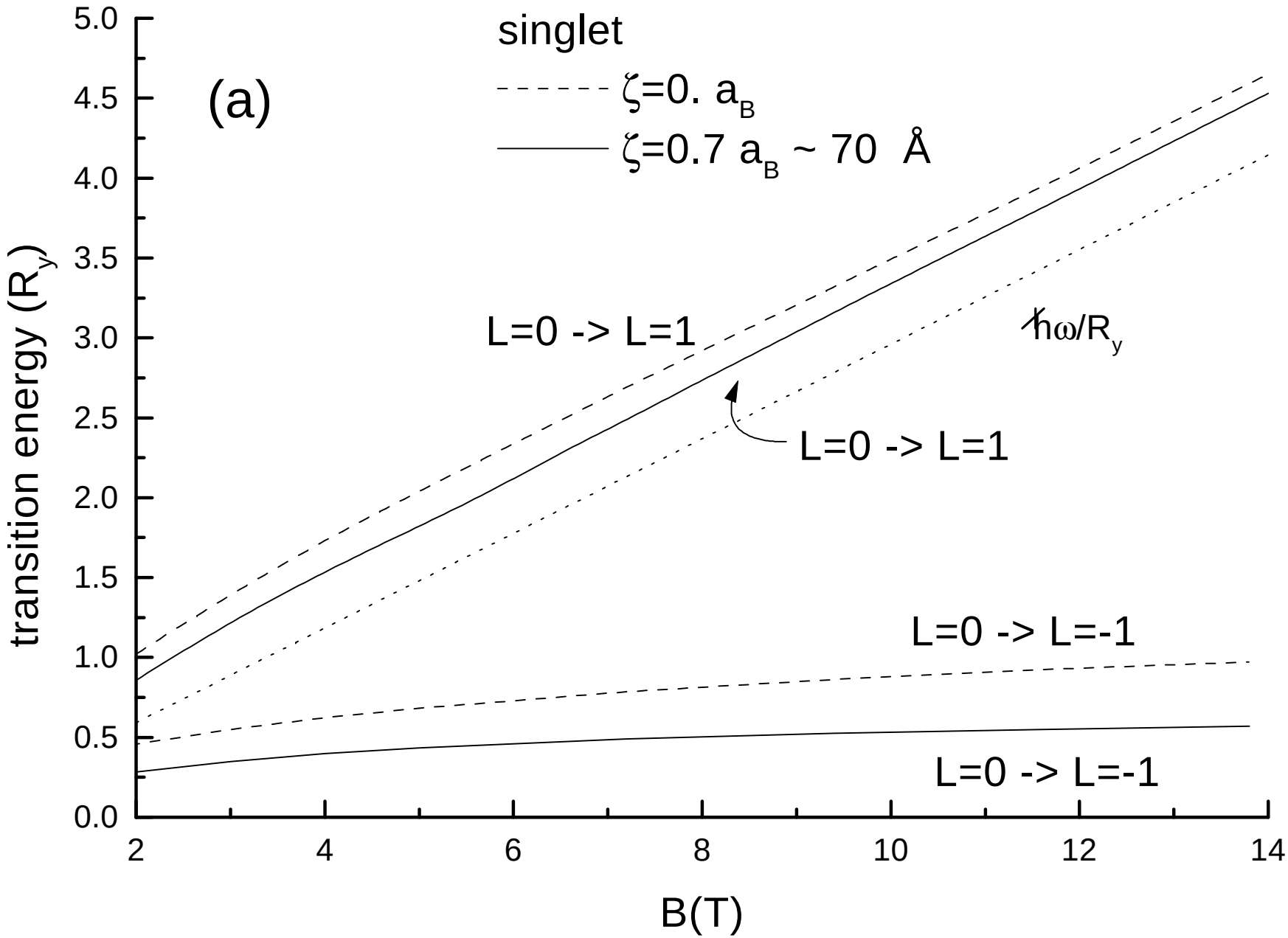

(a)
W=200 Å
L=0
ζ=0.7 a_B
ζ=0 a_B
B=15 T
B=5 T
<δ(ρ−|ρ_1−ρ_2|)>
ρ/a_B
0.00
0.05
0.10
0.15
0.20
0.0
0.5
1.0
1.5
2.0
2.5
3.0

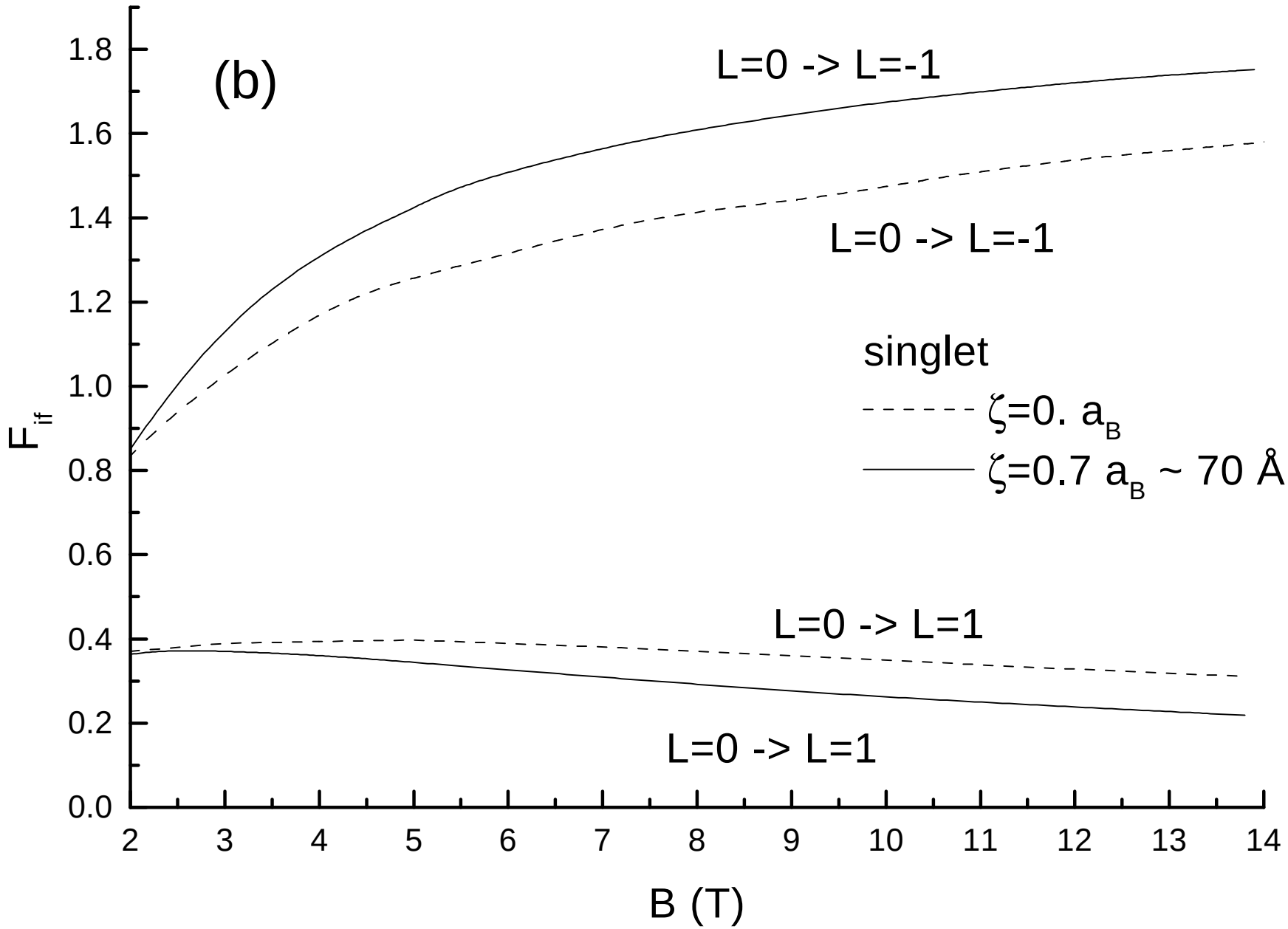

(b)
W=200 Å
L=-1
ζ=0.7 a_B
ζ=0 a_B
B=15 T
B=5 T
<δ(ρ−|ρ_1−ρ_2|)>
ρ/a_B
0.00
0.02
0.04
0.06
0.08
0.10
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0

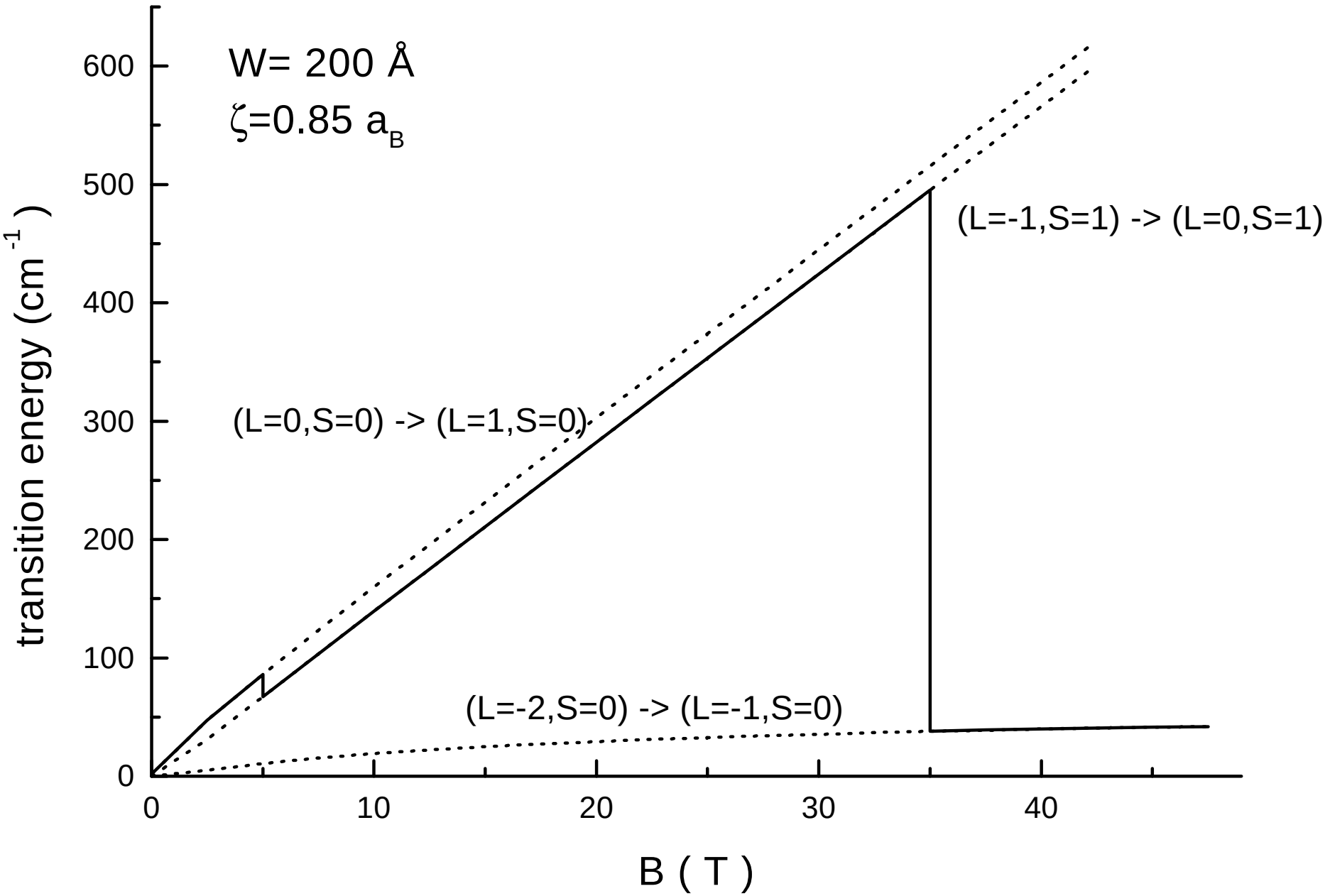

0.30
0.25
0.20
0.15
0.10
0.05
0.00
0
2
4
6
8
10
12
14
$E_b^{D^-}(R_y)$
γ
100 Å
ζ=.70a_B ~ 70 Å
L=0
L=-1
L=-2
L=-3
L=-4

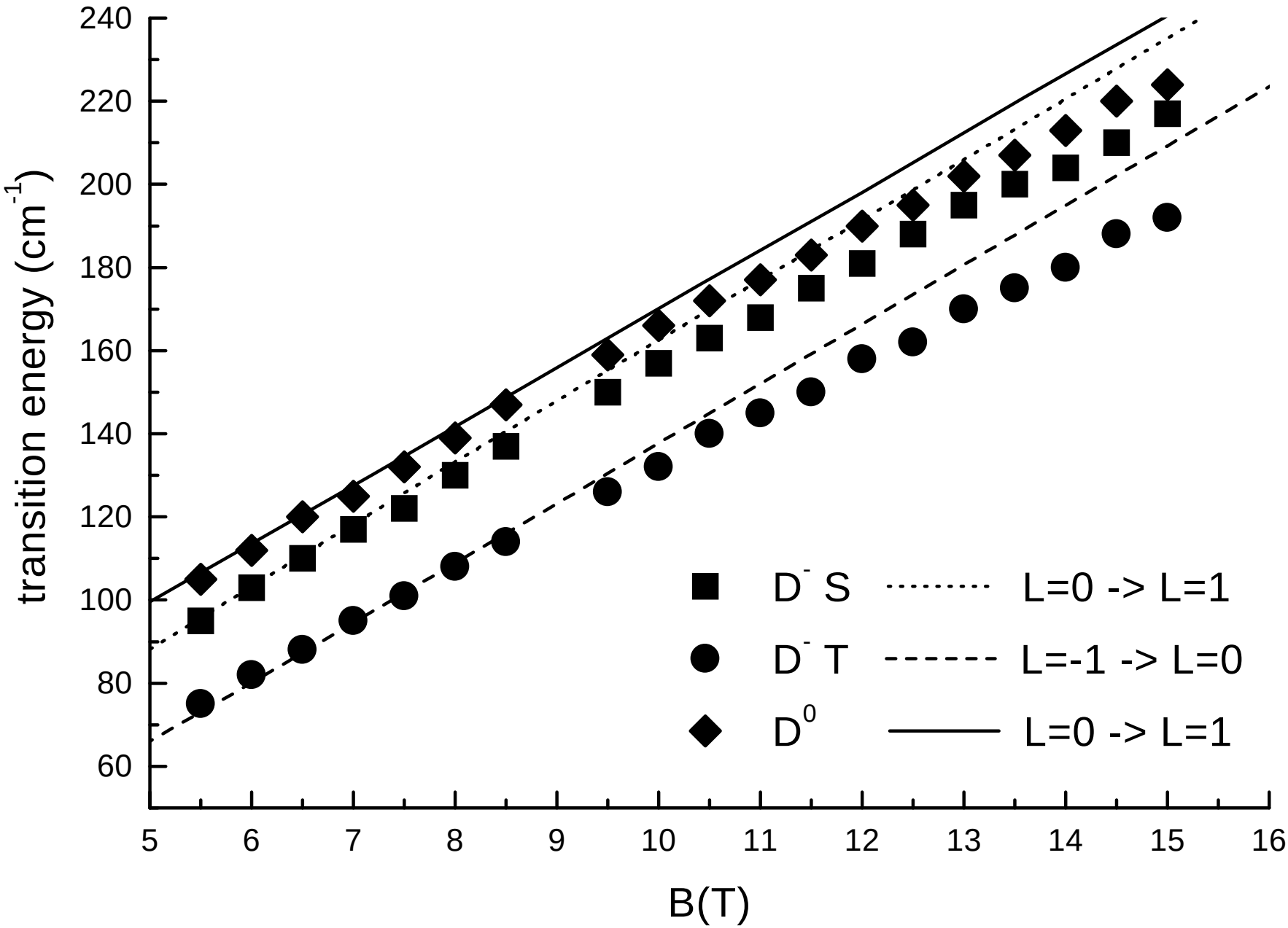

ζ (Å)
30
40
50
60
70
80
90
15.0
12.5
10.0
7.5
5.0
2.5
0.0
γc
100
80
60
40
20
0
Bc(T)
W= 100 Å
no bound-state
L=-3
triplet
L=-4
singlet
L=-2
singlet
L=-1 triplet
L=0 singlet
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
ζ/aB

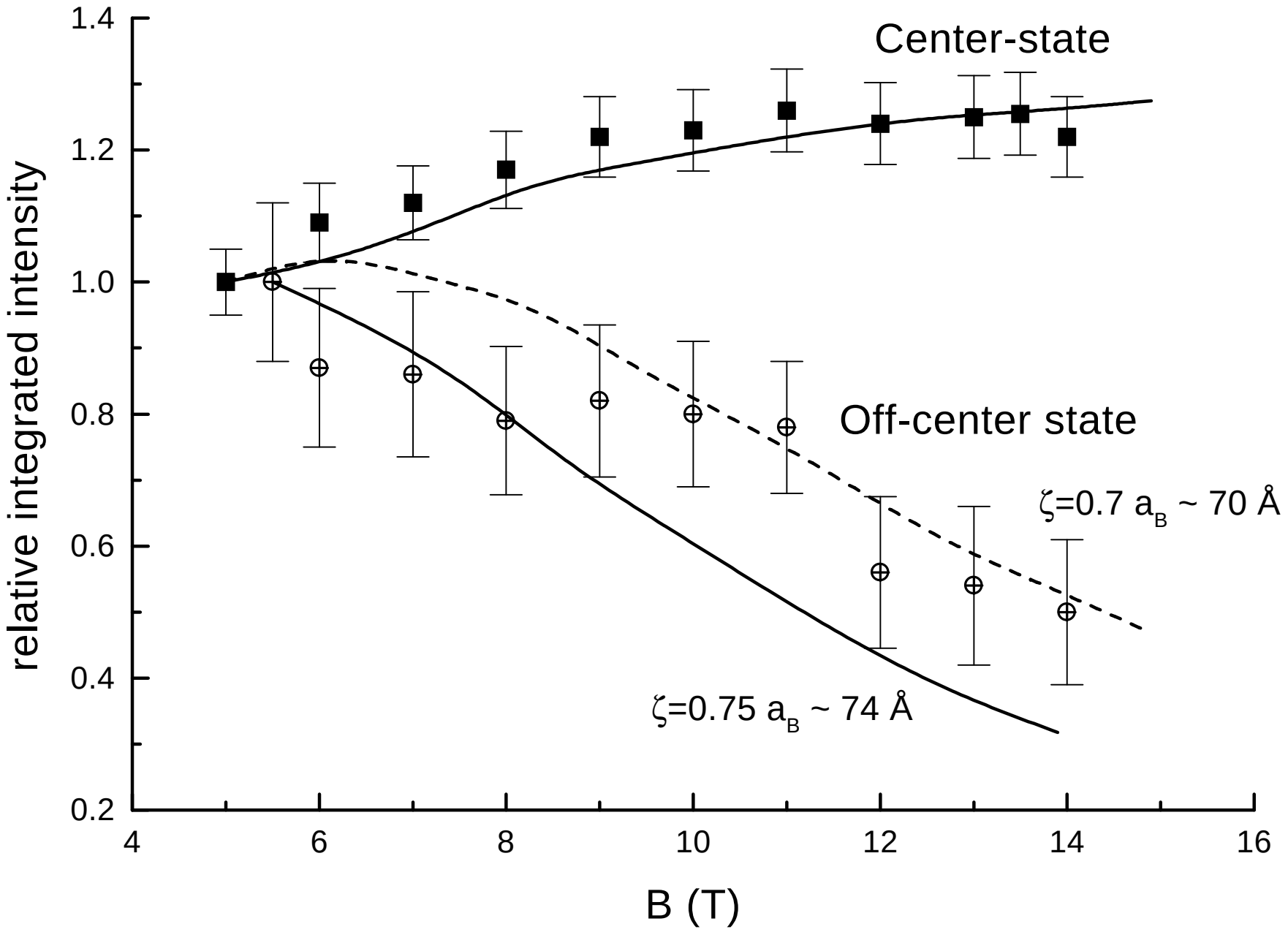

ζ=0.7a_B ~ 70 Å
no bound-states
L=-4 singlet
L=-3 triplet
L=-2 singlet
L=-1 triplet
L=0 singlet
γ_c
B_c (T)
W (Å)
20
18
16
14
12
10
8
6
4
2
0
-2
140
120
100
80
60
40
20
0
100
120
140
160
180
200


(a)
singlet
ζ=0. a_B
ζ=0.7 a_B ~ 70 Å
L=0 -> L=1
ħω/R_y
L=0 -> L=1
L=0 -> L=-1
L=0 -> L=-1
transition energy (R_y)
B(T)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
8
10
12
14


(b)
L=0 -> L=-1
L=0 -> L=-1
singlet
ζ=0. a_B
ζ=0.7 a_B ~ 70 Å
L=0 -> L=1
L=0 -> L=1
F_if
B (T)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2
3
4
5
6
7
8
9
10
11
12
13
14


W= 200 Å
ζ=0.85 a_B
(L=-1,S=1) -> (L=0,S=1)
(L=0,S=0) -> (L=1,S=0)
(L=-2,S=0) -> (L=-1,S=0)
transition energy (cm^-1)
B (T)
0
100
200
300
400
500
600
0
10
20
30
40


transition energy (cm-1)
240
220
200
180
160
140
120
100
80
60
5
6
7
8
9
10
11
12
13
14
15
16
B(T)
D- S
L=0 -> L=1
D- T
L=-1 -> L=0
D0
L=0 -> L=1


Center-state
Off-center state
ζ=0.7 a_B ~ 70 Å
ζ=0.75 a_B ~ 74 Å
relative integrated intensity
B (T)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
4
6
8
10
12
14
16